

CO2 solubility and composition data of food products stored in data warehouse structured by an ontology

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This dataset presents the values of CO₂ solubility at different temperatures and main compositional parameters (protein, fat, moisture, sugars and salt content) for food products from different categories: dairy products, fishes and meats. Due to its bacteriostatic effect, CO₂ is a key component for modified atmosphere packaging. However, the experimental determination of its solubility is long and costly. This dataset offers an exhaustive collection of state-of-the-art results, which can greatly benefit ongoing research. All the stakeholders of the food-engineering field can benefit from this for modelling gas transfer in food. These data could also serve as benchmark for other researchers dealing with characterization and modelling of CO₂ transfer in food.

It is the result of an extensive meta-analysis gathering the results of different major papers published on the domain on the period of 1980 to 2021, presenting the composition of 81 different food products corresponding to 362 solubility measures. Solubility data and their temperature of measurement were acquired through an extensive monitoring on the Web of Science (<https://www.webofscience.com/>) by three reviewers using the keywords “CO₂ solubility” and “Food” conducted twice a year over 2016 to 2021, which constituted a database of 21 references from 1980 to 2021.

For all measures, compositional data were added from the articles if available. In case of missing (or, in some cases, incomplete) information, the dataset was complemented using the MultiDB explorer tool [1] (<https://ico.iate.inra.fr/meatylab>), that compiles several diverse open-sourced databases (such as ANSES-CIQUAL, USDA). The composition (water, fat, proteins, sugar, salt) of the food product the closest to the one mentioned in the original article was used to fill in the database. The dataset was also enriched with CO₂ solubility measurements and their temperature on pure water and oil.

Data are stored as a knowledge graph structured by the @Web Matter Transfer ontology, which is dedicated to represent n-ary relations (i.e., relations to link multiple concepts together) in the field of mass transfer, especially gas (e.g. O₂ and CO₂), in food and packaging [2]. Two relations are defined: a first to link a food product to its solubility to CO₂, and a second to link the same food product to its nutritional composition. Moreover, values are structured such that they are always associated with a unit, which allows comparison between the different entries. The knowledge graph can be accessed manually through the @Web interface (<https://data.inrae.fr/dataverse/atweb>); it can also be directly queried using the SPARQL language in the accessible SPARQL endpoint (<https://ico.iate.inra.fr/fuseki/annotation/query>). All data from this dataset can be traced to their original source, guaranteeing a trackability of the different information, in accordance of the FAIR data principle.

[1] P. Buche, J. Cufi, S. Dervaux, S. Dibia, L. Ibanescu, A. Oudot, M. Weber, How to Manage Incompleteness of Nutritional Food Sources? A solution using FoodOn as pivot ontology, *Int. J. Agricul. Environ. Inform. Syst., IGI Global* 12 (4) (2021) 1–26, doi:10.4018/IJAEIS.20211001.0a4.

[2] V. Guillard, P. Buche, L. Menut, S. Dervaux, Matter Transfer Ontology, 2018. <https://doi.org/10.15454/NK24ID>.

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